

FILE 'REGISTRY' ENTERED AT 17:13:25 ON 15 MAY 2009

L1               STRUCTURE UPLOADED  
L2               0 S L1  
L3               STRUCTURE UPLOADED  
L4               0 S L3  
L5               7 S L3 SSS FULL

FILE 'ZCAPLUS' ENTERED AT 17:15:25 ON 15 MAY 2009

L6               9 S L5

=> file stnguide  
COST IN U.S. DOLLARS  
  
FULL ESTIMATED COST

SINCE FILE	TOTAL
ENTRY	SESSION
0.22	0.22

FILE 'STNGUIDE' ENTERED AT 17:13:21 ON 15 MAY 2009  
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FILE CONTAINS CURRENT INFORMATION.  
LAST RELOADED: May 11, 2009 (20090511/UP).

=> file registry  
COST IN U.S. DOLLARS  
  
FULL ESTIMATED COST

SINCE FILE	TOTAL
ENTRY	SESSION
0.07	0.29

FILE 'REGISTRY' ENTERED AT 17:13:25 ON 15 MAY 2009  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
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Property values tagged with IC are from the ZIC/VINITI data file  
provided by InfoChem.

STRUCTURE FILE UPDATES: 14 MAY 2009 HIGHEST RN 1146852-72-3  
DICTIONARY FILE UPDATES: 14 MAY 2009 HIGHEST RN 1146852-72-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

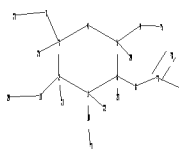
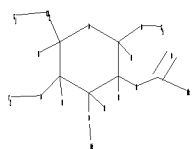
TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and  
predicted properties as well as tags indicating availability of  
experimental property data in the original document. For information  
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>  
Uploading C:\Program Files\STNEXP\Queries\10546132broad.str



```

chain nodes :
7  8  9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 27 29
33 35 36 37 38
ring nodes :
1  2  3  4  5  6
chain bonds :
1-10 1-22 2-11 2-21 3-7  3-25 5-9  5-24 6-8  6-23 7-27 8-33 9-35 10-37
11-29 12-13 12-19 13-14 13-18 15-16 16-17 17-20 33-36 33-38
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 1-10 2-3 2-11 3-4 4-5 5-6 5-9 6-8 7-27 8-33 9-35 10-37 11-29
16-17 33-36 33-38
exact bonds :
1-22 2-21 3-7 3-25 5-24 6-23 12-13 12-19 13-14 13-18 15-16 17-20

```

G1:H,Si,CH3

G2:H,P

G4

G5:[\*1],[\*2]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS

11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS

19:CLASS 20:CLASS

21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 27:CLASS 29:CLASS 33:CLASS

35:CLASS 36:CLASS

37:CLASS 38:CLASS

Generic attributes :

36:

Number of Carbon Atoms : 7 or more

37:

Number of Carbon Atoms : 7 or more

L1 STRUCTURE UPLOADED

=> s l1

SAMPLE SEARCH INITIATED 17:13:40 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 287 TO ITERATE

100.0% PROCESSED 287 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 4724 TO 6756

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> d l1

L1 HAS NO ANSWERS

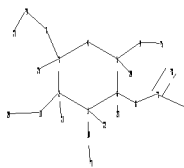
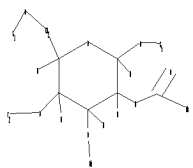
L1 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

=>

Uploading C:\Program Files\STNEXP\Queries\10546132broad2.str



chain nodes :

7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 27 29  
33 35 36 37 38 39

ring nodes :

1 2 3 4 5 6

chain bonds :

1-10 1-22 2-11 2-21 3-7 3-25 5-9 5-24 6-8 6-23 7-39 8-33 9-35 10-37  
11-29 12-13 12-19 13-14 13-18 15-16 16-17 17-20 27-39 33-36 33-38

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

1-2 1-6 1-10 2-3 2-11 3-4 4-5 5-6 5-9 6-8 8-33 9-35 10-37 11-29 16-17  
27-39 33-36 33-38

exact bonds :

1-22 2-21 3-7 3-25 5-24 6-23 7-39 12-13 12-19 13-14 13-18 15-16 17-20

G1:H,Si,CH3

G2:H,P

G4

G5:[\*1],[\*2]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS  
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS  
19:CLASS 20:CLASS  
21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 27:CLASS 29:CLASS 33:CLASS  
35:CLASS 36:CLASS  
37:CLASS 38:CLASS 39:CLASS

Generic attributes :

36:

Number of Carbon Atoms : 7 or more

37:

Number of Carbon Atoms : 7 or more

L3           STRUCTURE UPLOADED

=> s 13

SAMPLE SEARCH INITIATED 17:14:39 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED -           281 TO ITERATE

100.0% PROCESSED           281 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:   ONLINE   \*\*COMPLETE\*\*  
                          BATCH    \*\*COMPLETE\*\*

PROJECTED ITERATIONS:           4615 TO       6625

PROJECTED ANSWERS:               0 TO           0

L4           0 SEA SSS SAM L3

=> d 13

L3 HAS NO ANSWERS

L3           STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -   AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

=> s 13 sss full

FULL SEARCH INITIATED 17:15:06 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED -           5487 TO ITERATE

100.0% PROCESSED           5487 ITERATIONS

7 ANSWERS

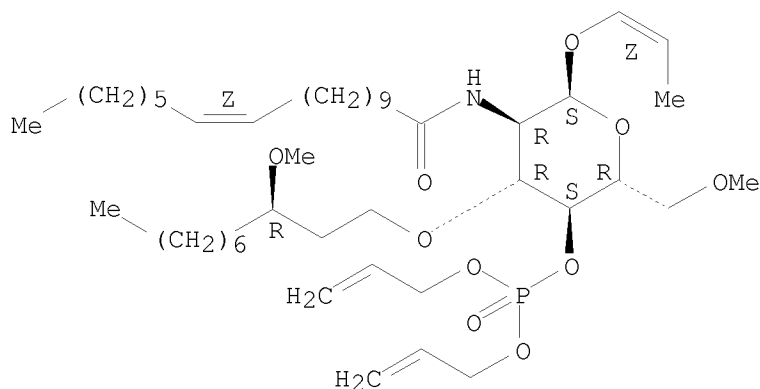
SEARCH TIME: 00.00.01

L5           7 SEA SSS FUL L3

=> d 15 scan

L5 7 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN  $\alpha$ -D-Glucopyranoside, (1Z)-1-propen-1-yl  
 2-deoxy-3-O-[(3R)-3-methoxydecyl]-6-O-methyl-2-[[ (11Z)-1-oxo-11-octadecen-  
 1-yl]amino]-, 4-(di-2-propen-1-yl phosphate)  
 MF C45 H82 N O10 P

Absolute stereochemistry.  
 Double bond geometry as shown.

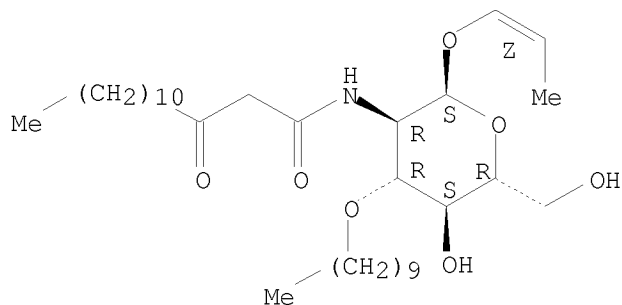


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):6

L5 7 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN  $\alpha$ -D-Glucopyranoside, (1Z)-1-propen-1-yl  
 3-O-decyl-2-deoxy-2-[(1,3-dioxotetradecyl)amino]-  
 MF C33 H61 N O7

Absolute stereochemistry.  
 Double bond geometry as shown.

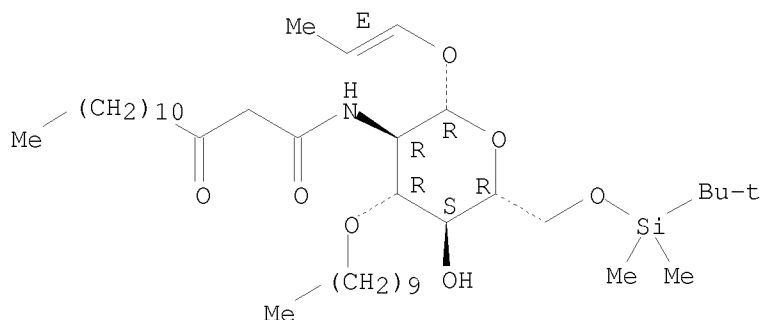


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L5 7 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN  $\beta$ -D-Glucopyranoside, (1E)-1-propen-1-yl  
 3-O-decyl-2-deoxy-6-O-[(1,1-dimethylethyl)dimethylsilyl]-2-[(1,3-

dioxotetradecyl)amino]-  
 MF C39 H75 N O7 Si

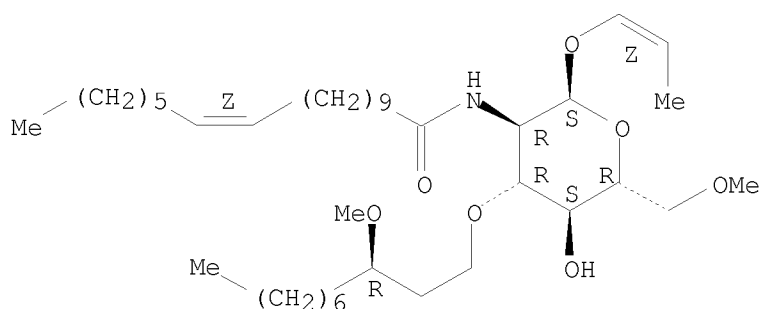
Absolute stereochemistry.  
 Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L5 7 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN  $\alpha$ -D-Glucopyranoside, (1Z)-1-propen-1-yl  
 2-deoxy-3-O-[(3R)-3-methoxydecyl]-6-O-methyl-2-[[ (11Z)-1-oxo-11-octadecen-  
 1-yl]amino]-  
 MF C39 H73 N O7

Absolute stereochemistry.  
 Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L5 7 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN  
 IN  $\alpha$ -D-Glucopyranose, 2-deoxy-3-O-[(3R)-3-methoxydecyl]-6-O-methyl-2-  
 [[ (11Z)-1-oxo-11-octadecen-1-yl]amino]-, 4-(di-2-propen-1-yl phosphate)  
 1-(2,2,2-trichloroethanimidate)  
 MF C44 H78 Cl3 N2 O10 P

Absolute stereochemistry.  
 Double bond geometry as shown.

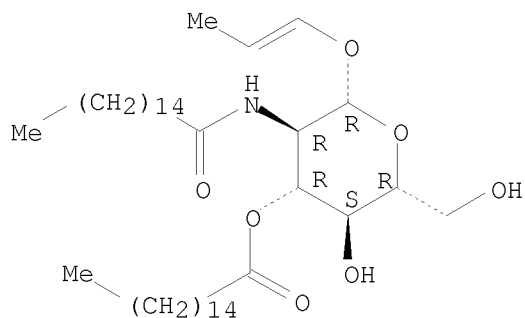




Absolute stereochemistry.  
Double bond geometry as shown.



Absolute stereochemistry.  
Double bond geometry unknown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=> file zcaplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

186.84

187.13

FILE 'ZCAPLUS' ENTERED AT 17:15:25 ON 15 MAY 2009

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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FILE COVERS 1907 - 15 May 2009 VOL 150 ISS 21

FILE LAST UPDATED: 14 May 2009 (20090514/ED)

REVISED CLASS FIELDS (/NCL) LAST RELOADED: Feb 2009

USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Feb 2009

ZCAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 15

L6

9 L5

=> d 16 1-9 ti abs bib hitstr

L6 ANSWER 1 OF 9 ZCAPLUS COPYRIGHT 2009 ACS on STN

TI Sodium salt of glucosamine disaccharide compound, method for producing the same, and use of the same

GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB There are disclosed a sodium salt represented by the average formula (I; m1, n1, m2 and n2 independently represent 0 or a pos. number not more than 2, while satisfying  $m1 + n1 = 2$ ,  $m2 + n2 = 2$ ,  $0 < m1 + m2 < 4$  and  $0 < n1 + n2 < 4$ .) and a method for producing such a sodium salt. There is also a decomposition suppressing method which enables to have a sodium salt represented by the average formula I coexistent with a sodium salt represented by the general formula II below. This method enables to improve long-term stability of a sodium salt represented by the general formula II which is effective for the prevention and/or treatment of septicemia caused by gram pos. bacteria, in particular endotoxin shock. Thus, a DEAE column main fraction containing 6.0 g disaccharide free acid (III) (preparation given) and

4.80

weight% Na and 942.8 L MeOH were stirred in a 4 L flask at 25°, treated with 0.2 N NaOH/MeOH solution (15.2 mL), stirred overnight, filtered, and treated dropwise with 270 mL acetone at 25°. The precipitate was removed by filtration and dried in vacuo to give III.3.67 Na. When III.3.67 Na was stored in a screw-cap bottle at 25° for 30 days, impurities A, B, and C were formed at a rate of 0.072, 0.267, and 0.072 %/mo, resp., vs. 0.729, 3.117, and 0.033 %/mo, resp., for III.4.06Na.

AN 2008:636616 ZCAPLUS <<LOGINID::20090515>>

DN 149:10241

TI Sodium salt of glucosamine disaccharide compound, method for producing the same, and use of the same

IN Sakurai, Shin; Furukawa, Ken; Matsuo, Kimihiro; Tagami, Kenichi

PA Eisai R & D Management Co., Ltd., Japan

SO PCT Int. Appl., 46pp.

CODEN: PIXXD2

DT Patent

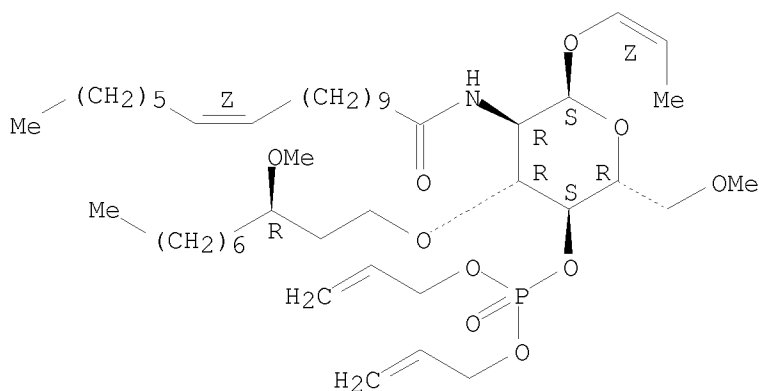
LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2008062842	A1	20080529	WO 2007-JP72579	20071121
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	RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	US 20080227991	A1	20080918	US 2007-984770	20071121
PRAI	JP 2006-315020	A	20061122		
	US 2006-860483P	P	20061122		

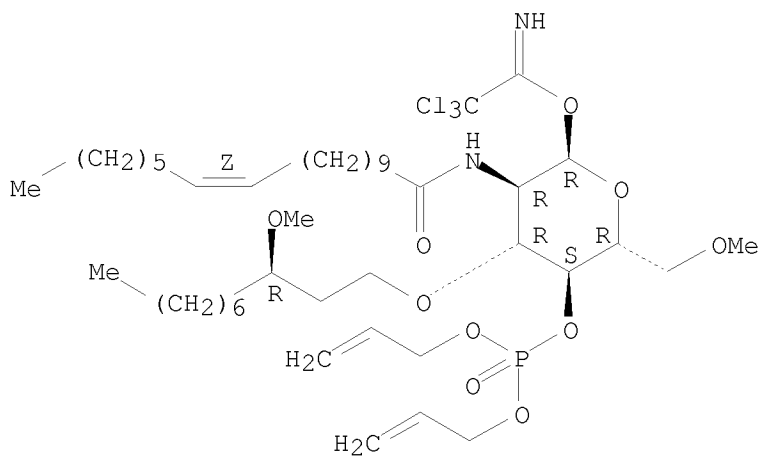
IT 748165-18-6P 748165-20-0P  
 RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (intermediate; preparation of sodium salt of glucosamine disaccharide compound  
 with storage stability, method for producing it, and its use for prevention and/or treatment of endotoxin shock)  
 RN 748165-18-6 ZCAPLUS  
 CN  $\alpha$ -D-Glucopyranoside, (1Z)-1-propen-1-yl  
 2-deoxy-3-O-[(3R)-3-methoxydecyl]-6-O-methyl-2-[[[(11Z)-1-oxo-11-octadecen-1-yl]amino]-, 4-(di-2-propen-1-yl phosphate) (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry as shown.



RN 748165-20-0 ZCAPLUS  
 CN  $\alpha$ -D-Glucopyranose, 2-deoxy-3-O-[(3R)-3-methoxydecyl]-6-O-methyl-2-[[[(11Z)-1-oxo-11-octadecen-1-yl]amino]-, 4-(di-2-propen-1-yl phosphate) 1-(2,2,2-trichloroethanimidate) (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry as shown.



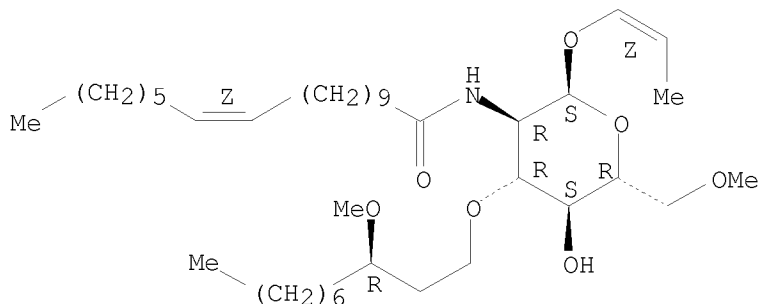
IT 748165-17-5  
 RL: RCT (Reactant); RACT (Reactant or reagent)

stability, method for producing it, and its use for prevention and/or treatment of endotoxin shock)

CN  $\alpha$ -D-Glucopyranoside, (1Z)-1-propen-1-yl

1-vllamino]- (CA INDEX NAME)

Double bond geometry as shown.

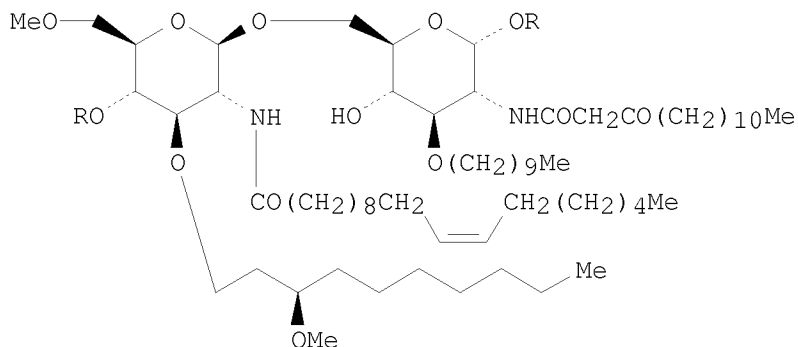


RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE.FORMAT

L6 ANSWER 2 OF 9 ZCAPLUS COPYRIGHT 2009 ACS on STN

## TI Process for production of lipid A analogue

GI



I

AB There is disclosed a process for producing 3-O-decyl-2-deoxy-6-O-[2-deoxy-3-O-[(3R)-3-methoxydecyl]-6-O-methyl-2-[[ (11Z)-1-oxo-11-octadecenyl]amino]-4-O-phosphono-β-D-glucopyranosyl]-2-[(1,3-dioxotetradecyl)amino]-α-D-glucopyranose 1-(dihydrogen phosphate) (known as eritoran) tetrasodium salt (I; R = PO<sub>3</sub>Na<sub>2</sub>) which is useful as an active ingredient of a pharmaceutical or an intermediate for the synthesis thereof. A process for producing the compound I (R = PO<sub>3</sub>Na<sub>2</sub>) comprises the key steps of reacting a compound represented by the formula I [R = P(O)(OCH<sub>2</sub>CH:CH<sub>2</sub>)<sub>2</sub>] with a palladium catalyst in the presence of a

nucleophilic agent (deallylation) and treating the product with a sodium source (sodium salt formation). This process is environment-friendly and excellent in safety, operationability, and reproducibility. Thus, a solution of 101.6 g I [R = P(O)(OCH<sub>2</sub>CH:CH<sub>2</sub>)<sub>2</sub>] in 203 mL THF was added to a mixture of Meldrum's acid 70.49, palladium acetate 2.93, and PPh<sub>3</sub> 51.3 g and the resulting mixture was stirred at 32° for 2 h and at 30° for 4 h, treated with 250 mL MeOH, and concentrated under reduced pressure to give a residue (466.7 g). The residue was dissolved in 4,570 mL MeOH at 40°, treated with 5.55 g trimercaptotriazine, stirred overnight at room temperature, and filtered to remove the precipitated

trimercaptotriazine-palladium

complex, followed by washing the precipitate with MeOH to give a combined filtrate (4,330 g). The filtrate (3,908.2 mL) was concentrated under reduced pressure to give a residue (440.9 g) which was treated with 450 mL acetone, concentrated under reduced pressure, treated again with 450 mL

acetone,

and concentrated under reduced pressure. The residue was refrigerated overnight, treated with 1,800 mL acetone, warmed to 40°, stirred for 1.5 h, air-cooled, stirred at ≥30° for 1.5 h, and filtered to give, after washing with acetone and drying at 35-40° under reduced pressure, 74.2% eritoran (free acid form) which was treated with 0.1 N aqueous NaOH solution to give eritoran tetrasodium salt.

AN 2007:257680 ZCAPLUS <<LOGINID::20090515>>

DN 146:317153

TI Process for production of lipid A analogue

IN Tagami, Katsuya; Sato, Keizo; Matsuo, Kimihiro; Abe, Taichi; Haga, Toyokazu

PA Eisai R & D Management Co., Ltd., Japan

SO PCT Int. Appl., 69pp.

CODEN: PIXXD2

DT Patent

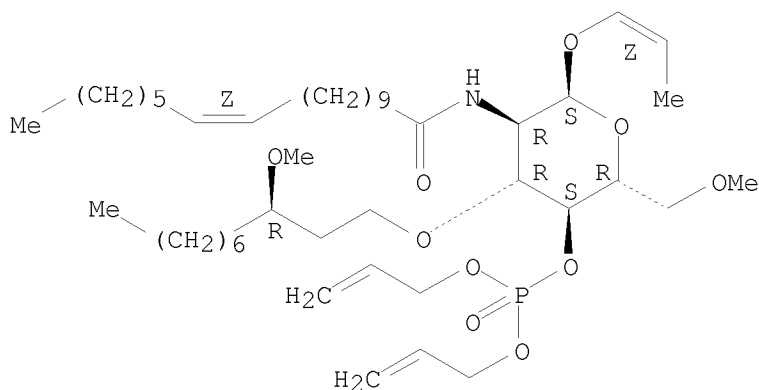
LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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	RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	AU 2006285926	A1	20070308	AU 2006-285926	20060829
	CA 2620027	A1	20070308	CA 2006-2620027	20060829
	EP 1939209	A1	20080702	EP 2006-796921	20060829
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	KR 2008039374	A	20080507	KR 2008-700572	20080109
	CN 101238140	A	20080806	CN 2006-80027144	20080124
	IN 2008CN01457	A	20081128	IN 2008-CN1457	20080325
PRAI	US 2005-712431P	P	20050831		
	JP 2005-253044	A	20050901		
	WO 2006-JP316941	W	20060829		
OS	CASREACT 146:317153				

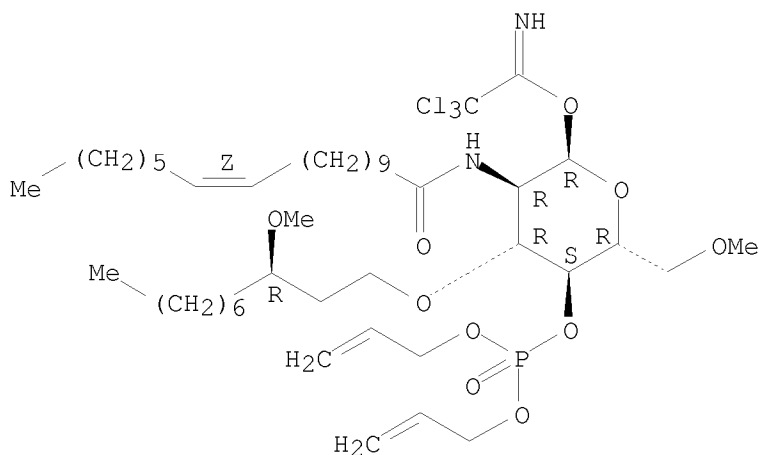
IT 748165-18-6P 748165-20-0P  
 RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (process for production of lipid A analog (eritoran) via palladium-catalyzed deallylation of eritoran diallyl ester and formation of sodium salt)  
 RN 748165-18-6 ZCAPLUS  
 CN  $\alpha$ -D-Glucopyranoside, (1Z)-1-propen-1-yl 2-deoxy-3-O-[(3R)-3-methoxydecyl]-6-O-methyl-2-[[ (11Z)-1-oxo-11-octadecen-1-yl]amino]-, 4-(di-2-propen-1-yl phosphate) (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry as shown.



RN 748165-20-0 ZCAPLUS  
 CN  $\alpha$ -D-Glucopyranose, 2-deoxy-3-O-[(3R)-3-methoxydecyl]-6-O-methyl-2-[[ (11Z)-1-oxo-11-octadecen-1-yl]amino]-, 4-(di-2-propen-1-yl phosphate) 1-(2,2,2-trichloroethanimidate) (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry as shown.



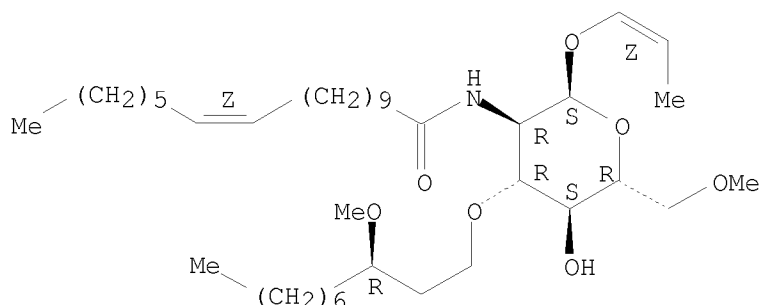
IT 748165-17-5  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (process for production of lipid A analog (eritoran) via

palladium-catalyzed deallylation of eritoran diallyl ester and  
formation of sodium salt)

RN 748165-17-5 ZCAPLUS

CN  $\alpha$ -D-Glucopyranoside, (1Z)-1-propen-1-yl  
2-deoxy-3-O-[(3R)-3-methoxydecyl]-6-O-methyl-2-[[ (11Z)-1-oxo-11-octadecen-  
1-yl]amino]- (CA INDEX NAME)

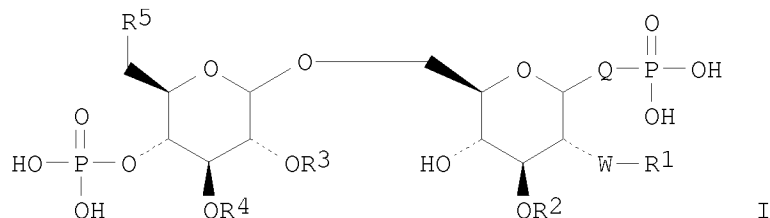
Absolute stereochemistry.  
Double bond geometry as shown.



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 9 ZCAPLUS COPYRIGHT 2009 ACS on STN

TI Preparation of glucose lipid A analogs inhibiting macrophage activity  
GI



AB Title compds. I [Q = -O-, alkylene, -O-alkylene, etc.; W = -O- or -NH-; when W is -NH-, R1 is alkanoyl, alkenoyl, alkynoyl. (wherein alkanoyl, alkenoyl and alkynoyl are optionally substituted with halo, hydroxy, oxo, etc.); each R1 (when W is -O-), R2, R3, and R4 is H, alkyl, alkenyl, etc. (wherein alkyl and alkenyl are optionally substituted with halo, hydroxy, oxo, etc.); R5 = H, halo, hydroxy, etc.] and their pharmacol. acceptable salts were prepared For example, phosphono 3-O-decyl-2-deoxy-6-O-[3-O-[(R)-3-methoxydecyl]-6-O-methyl-2-O-[(Z)-11-octadecenoyl]-4-O-phosphono- $\beta$ -D-glucopyranosyl]-2-(3-oxotetradecanoylamino)- $\alpha$ -D-glucopyranoside (II) was prepared from 1,2:5,6-di-O-isopropylidene- $\alpha$ -D-glucofuranose in 18 steps. In human TNF $\alpha$  production inhibition assays, the IC50 value of compound II was 0.49 nM. Compds. I are claimed useful for the treatment of inflammation, autoimmune diseases, etc.

AN 2007:167289 ZCAPLUS <<LOGINID::20090515>>



DN 146:252059  
 TI Preparation of glucose lipid A analogs inhibiting macrophage activity  
 IN Shiozaki, Masao; Shimozato, Ryuichi  
 PA Sankyo Co., Ltd., Japan  
 SO Jpn. Kokai Tokkyo Koho, 86pp.  
 CODEN: JKXXAF

DT Patent  
 LA Japanese

FAN.CNT 1

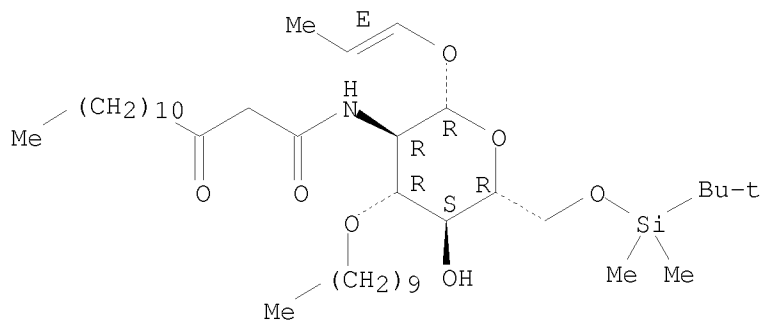
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 2007039450	A	20070215	JP 2006-187298	20060707
PRAI	JP 2005-199518	A	20050708		
OS	MARPAT 146:252059				
IT	859508-28-4P				

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of glucose lipid analogs for treatment of inflammation and autoimmune diseases)

RN 859508-28-4 ZCAPLUS

CN  $\beta$ -D-Glucopyranoside, (1E)-1-propen-1-yl  
 3-O-decyl-2-deoxy-6-O-[(1,1-dimethylethyl)dimethylsilyl]-2-[(1,3-dioxotetradecyl)amino]- (CA INDEX NAME)

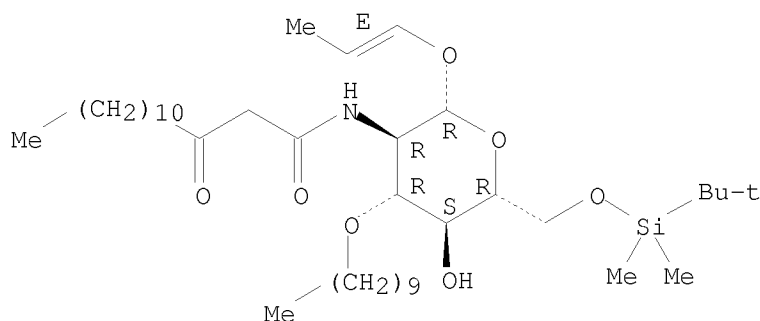
Absolute stereochemistry.  
 Double bond geometry as shown.



L6 ANSWER 4 OF 9 ZCAPLUS COPYRIGHT 2009 ACS on STN  
 TI Syntheses of glucose-containing E5564 analogs and their LPS-antagonistic activities  
 AB Lipid A analogs containing a glucose moiety on their non-reducing end were synthesized, and their LPS-antagonistic activities were measured. The inhibitory activities (IC50) on LPS-induced TNF $\alpha$  production of title aminodeoxy disaccharides toward human whole blood cells were 0.46-1.11 nM. Inhibitory doses (ID50) of these compds. on TNF $\alpha$  production induced by co-injection of galactosamine and LPS in C3H/HeN mice were measured. The ID50 values of these compds. were 0.20-1.08 and <0.2 mg/kg. Moreover, C3H/HeN mice preinjected with compds. were protected from lethality induced by co-injection of galactosamine and LPS. Out of eight mice preinjected with 1 mg/kg of title compds. five-eight mice were protected.  
 AN 2005:1299295 ZCAPLUS <<LOGINID::20090515>>  
 DN 144:171174  
 TI Syntheses of glucose-containing E5564 analogs and their LPS-antagonistic activities  
 AU Shiozaki, Masao; Doi, Hiromi; Tanaka, Daisuke; Shimozato, Takaichi; Kurakata, Shin-ichi

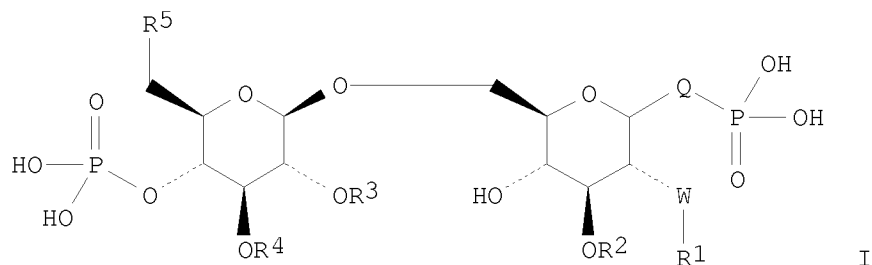
CS Chemistry Department, Chemtech Labo, Inc., Hiromachi 1-2-58, Shinagawa-ku,  
Tokyo, 140-8710, Japan  
SO Tetrahedron (2005), Volume Date 2006, 62(1), 205-225  
CODEN: TETRAB; ISSN: 0040-4020  
PB Elsevier B.V.  
DT Journal  
LA English  
OS CASREACT 144:171174  
IT 859508-28-4P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(syntheses of glucose-containing E5564 analogs and their LPS-antagonistic  
activities)  
RN 859508-28-4 ZCAPLUS  
CN  $\beta$ -D-Glucopyranoside, (1E)-1-propen-1-yl  
3-O-decyl-2-deoxy-6-O-[(1,1-dimethylethyl)dimethylsilyl]-2-[(1,3-  
dioxotetradecyl)amino]- (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.



RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 9 ZCAPLUS COPYRIGHT 2009 ACS on STN  
TI preparation of levulose glucoselipid A derivatives as TNF $\alpha$   
production inhibitors  
GI



AB Title compds. I [Q = O, etc.; W = O, NH; R<sup>1</sup> = (un)substituted alkanoyl,  
etc. with the proviso that if W = NH; R<sup>1</sup> (with the proviso that if W = O),

R2, R3, R4 = H, (un)substituted alkyl, etc.; R5 = H, halo, etc.] were prepared For example, phosphorylation of 4-O-(allyloxycarbonyl)-3-O-decyl-2-deoxy-6-O-[4-O-diallylphosphono-3-O-[(R)-3-methoxydecyl]-6-O-methyl-2-O-[(Z)-11-octadecenoyl]- $\beta$ -D-glucopyranosyl]-2-(3-oxotetradecanoylamino)- $\alpha$ -D-glucopyranoside, e.g., prepared from 1,2:5,6-di-O-isopropylidene- $\alpha$ -D-glucofuranose in 15 steps, with diallyl diisopropylphosphoramidate followed by deallylation using Pd(PPh<sub>3</sub>)<sub>4</sub> afforded phosphono 3-O-decyl-2-deoxy-6-O-[3-O-[(R)-3-methoxydecyl]-6-O-methyl-2-O-[(Z)-11-octadecenoyl]-4-O-phosphono- $\beta$ -D-glucopyranosyl]-2-(3-oxotetradecanoylamino)- $\alpha$ -D-glucopyranoside (II). In TNF $\alpha$  production inhibition assays, the IC<sub>50</sub> value of compound II was 0.49 nM. Compds. I are claimed useful for the treatment of inflammation, septicemia, etc.

AN 2005:638895 ZCAPLUS <<LOGINID::20090515>>

DN 143:153644

TI preparation of levulose glucoselipid A derivatives as TNF $\alpha$  production inhibitors

IN Shiozaki, Masao; Shimoizato, Takaichi

PA Sankyo Company, Limited, Japan

SO PCT Int. Appl., 156 pp.

CODEN: PIXXD2

DT Patent

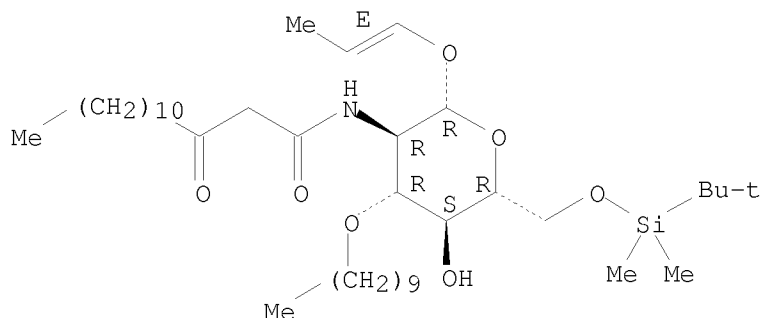
LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005066193	A1	20050721	WO 2005-JP434	20050107
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA 2552218	A1	20050721	CA 2005-2552218	20050107
	JP 2005220130	A	20050818	JP 2005-2028	20050107
	EP 1702926	A1	20060920	EP 2005-703673	20050107
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS				
	CN 1930180	A	20070314	CN 2005-80007429	20050107
	BR 2005006671	A	20070515	BR 2005-6671	20050107
	IN 2006KN01892	A	20070511	IN 2006-KN1892	20060706
	MX 2006007822	A	20060926	MX 2006-7822	20060707
	KR 2006121293	A	20061128	KR 2006-713689	20060707
	US 20090062214	A1	20090305	US 2008-585640	20080929
PRAI	JP 2004-2902	A	20040108		
	WO 2005-JP434	W	20050107		
OS	MARPAT 143:153644				
IT	859508-28-4P				
	RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)				
	(preparation of levulose glucoselipid A derivs. as TNF $\alpha$ production inhibitors for treatment of inflammation, septicemia, etc.)				
RN	859508-28-4 ZCAPLUS				
CN	$\beta$ -D-Glucopyranoside, (1E)-1-propen-1-yl				
	3-O-decyl-2-deoxy-6-O-[(1,1-dimethylethyl)dimethylsilyl]-2-[(1,3-				

dioxotetradecyl)amino]- (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.



RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 6 OF 9 ZCAPLUS COPYRIGHT 2009 ACS on STN  
TI Reagents and methods for preparing lipopolysaccharides antagonist B1287  
and stereoisomers thereof for treatment of various forms of septic shock  
GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The present invention provides methods for preparing lipopolysaccharides (LPS) antagonist lipo-disaccharide B1287 and stereoisomers thereof, which compds. are useful as in the prophylactic and affirmative treatment of endotoxemia including sepsis, septicemia and various forms of septic shock (no biol. data). Also provided are synthetic intermediates useful for implementing the inventive methods. Thus, lipo-disaccharide B1287 I was prepared for treatment of various forms of septic shock.

AN 2004:718552 ZCAPLUS <<LOGINID::20090515>>

DN 141:225771

TI Reagents and methods for preparing lipopolysaccharides antagonist B1287 and stereoisomers thereof for treatment of various forms of septic shock

IN Fan, Rulin

PA Eisai Co, Ltd., Japan

SO PCT Int. Appl., 175 pp.

CODEN: PIXXD2

DT Patent

LA English

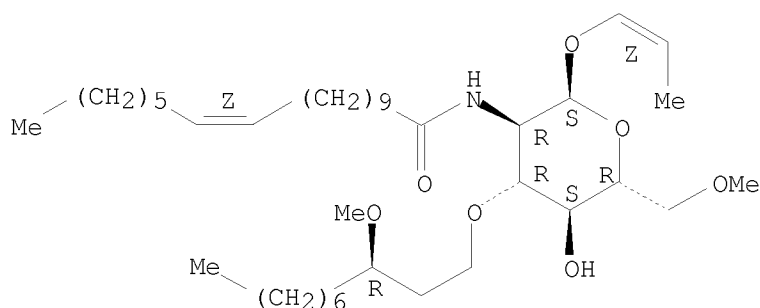
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004074303	A2	20040902	WO 2004-US4921	20040218
	WO 2004074303	A3	20041229		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN,

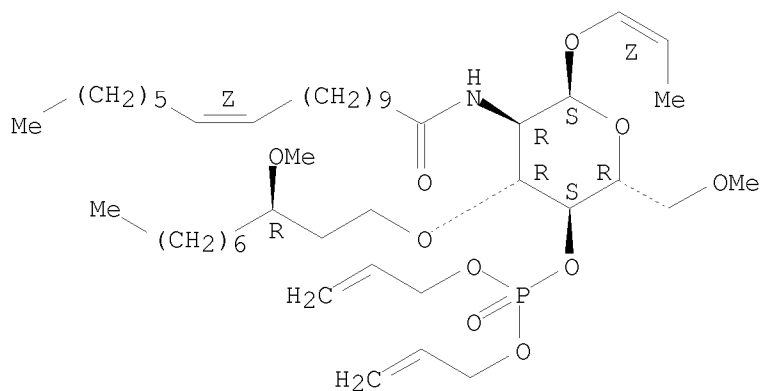
GQ, GW, ML, MR, NE, SN, TD, TG  
 JP 2006518394 T 20060810 JP 2006-503710 20040218  
 US 20060160999 A1 20060720 US 2005-546132 20051212  
 PRAI US 2003-448839P P 20030220  
 WO 2004-US4921 W 20040218  
 OS CASREACT 141:225771; MARPAT 141:225771  
 IT 748165-17-5P 748165-18-6P 748165-20-0P  
 748165-24-4P 748165-25-5P  
 RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic  
 preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (reagents and methods for preparing lipopolysaccharides antagonist b and  
 stereoisomers thereof for treatment of various forms of septic shock)  
 RN 748165-17-5 ZCAPLUS  
 CN  $\alpha$ -D-Glucopyranoside, (1Z)-1-propen-1-yl  
 2-deoxy-3-O-[(3R)-3-methoxydecyl]-6-O-methyl-2-[[ (11Z)-1-oxo-11-octadecen-  
 1-yl]amino]- (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry as shown.



RN 748165-18-6 ZCAPLUS  
 CN  $\alpha$ -D-Glucopyranoside, (1Z)-1-propen-1-yl  
 2-deoxy-3-O-[(3R)-3-methoxydecyl]-6-O-methyl-2-[[ (11Z)-1-oxo-11-octadecen-  
 1-yl]amino]-, 4-(di-2-propen-1-yl phosphate) (CA INDEX NAME)

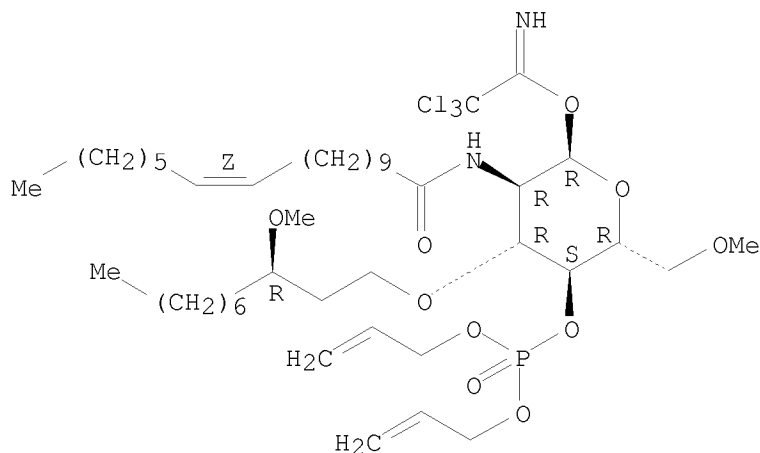
Absolute stereochemistry.  
 Double bond geometry as shown.



RN 748165-20-0 ZCAPLUS  
 CN  $\alpha$ -D-Glucopyranose, 2-deoxy-3-O-[(3R)-3-methoxydecyl]-6-O-methyl-2-

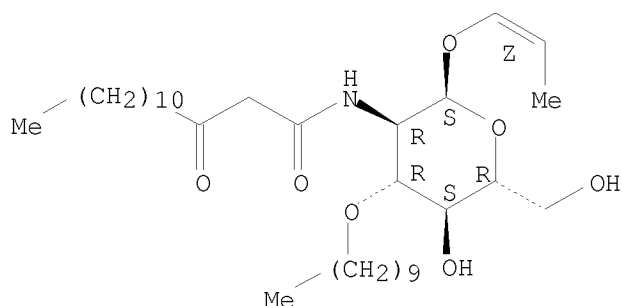
[[ (11Z)-1-oxo-11-octadecen-1-yl]amino]-, 4-(di-2-propen-1-yl phosphate)  
1-(2,2,2-trichloroethanimidate) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.



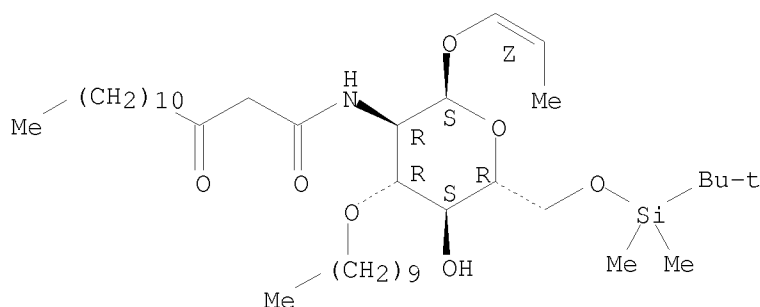
RN 748165-24-4 ZCAPLUS  
CN  $\alpha$ -D-Glucopyranoside, (1Z)-1-propen-1-yl  
3-O-decyl-2-deoxy-2-[(1,3-dioxotetradecyl)amino]- (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.



RN 748165-25-5 ZCAPLUS  
CN  $\alpha$ -D-Glucopyranoside, (1Z)-1-propen-1-yl  
3-O-decyl-2-deoxy-6-O-[(1,1-dimethylethyl)dimethylsilyl]-2-[(1,3-  
dioxotetradecyl)amino]- (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.



RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 7 OF 9 ZCAPLUS COPYRIGHT 2009 ACS on STN

TI Disaccharide

GI For diagram(s), see printed CA Issue.

AB Disaccharides I (R = alkyl, hydroxyalkyl or protected hydroxy alkyl of 7-19 C atoms; R1 = allyl, benzyl, 1-propenyl, trichloroethyl; R2 = H, RCO; R3 = allyl, crotyl, MeOCH2CH2OCH2, MeSCH2, benzyl; R4 = H, ClCH2CO,  $\beta$ -benzoylpropionyl), useful in the preparation of lipid A analogs, were prepared via coupling of the component monosaccharides by oxazoline method. Thus, I [RCO = palmitoyl, R1 = R3 = benzyl, R2 = palmitoyl, R4 = (Cl3CCH2O)2P(O)] was prepared in several steps starting from allyl and benzyl 3,4,6-tri-O-acetyl-2-deoxy-2-palmitamido- $\beta$ -D-glucopyranoside.

AN 1985:422874 ZCAPLUS <<LOGINID::20090515>>

DN 103:22874

OREF 103:3791a,3794a

TI Disaccharide

IN Anderson, Laurens; Nashed, Mina A.

PA Wisconsin Alumni Research Foundation, USA

SO U.S., 14 pp. Cont.-in-part of U.S. Ser. No. 248,692, abandoned.

CODEN: USXXAM

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4495346	A	19850122	US 1982-433055	19821006
PRAI	US 1981-248692	A2	19810330		
OS	MARPAT 103:22874				
IT	84766-03-0P				

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

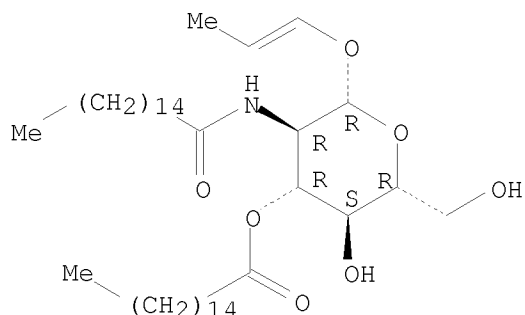
(preparation and glycosylation of, with (glucopyrano)oxazoline derivative)

RN 84766-03-0 ZCAPLUS

CN  $\beta$ -D-Glucopyranoside, 1-propen-1-yl  
2-deoxy-2-[(1-oxohexadecyl)amino]-, 3-hexadecanoate (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.



RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and reaction of, with (glucopyrano)oxazoline deriv.

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 8 OF 9 ZCAPLUS COPYRIGHT 2009 ACS on STN

TI The convergent approach to the synthesis of lipid A and its analogs

GI For diagram(s), see printed CA Issue.

AB A multistep preparation of disaccharide I (R = palmitoyl) and several other lipid A analogs are described.

AN 1984:103782 ZCAPLUS <<LOGINID::20090515>>

DN 100:103782

OREF 100:15789a,15792a

TI The convergent approach to the synthesis of lipid A and its analogs

AU Anderson, Laurens; Nashed, Mina A.

CS Coll. Agric. Life Sci., Univ. Wisconsin, Madison, WI, 53706, USA

SO ACS Symposium Series (1983), 231(Bact. Lipopolysaccharides), 255-75

CODEN: ACSMC8; ISSN: 0097-6156

DT Journal

LA English

IT 84766-03-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

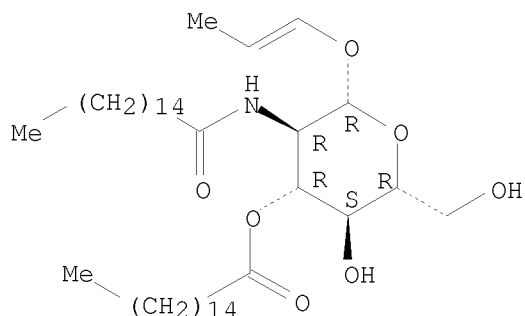
(preparation and glycosylation of, with glucosamine phosphate derivative)

RN 84766-03-0 ZCAPLUS

CN  $\beta$ -D-Glucopyranoside, 1-propen-1-yl  
2-deoxy-2-[(1-oxohexadecyl)amino]-, 3-hexadecanoate (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.





L6 ANSWER 9 OF 9 ZCAPLUS COPYRIGHT 2009 ACS on STN  
 TI Iodine as a reagent for the ready hydrolysis of prop-1-enyl glycosides,  
 for their conversion into oxazolines  
 GI For diagram(s), see printed CA Issue.  
 AB 1-Propenyl glycosides were readily hydrolyzed to free sugars by iodine in  
 aqueous oxolane. E.g., treatment of glycoside I (R = CH:CHMe) (II) with  
 iodine in 4:1 oxolane-H<sub>2</sub>O at room temperature for 5 min gave I (R = H). On  
 similar treatment in the presence of 1,5-diazabicyclo[5.4.0]undec-5-ene  
 (III), 1-propenyl  $\beta$ -glycosides of N-acylglucosamines cyclized to  
 oxazoline derivs. E.g., treatment of II with iodine in dry dioxolane  
 containing III for .apprx.5 min gave >95% IV.  
 AN 1983:107634 ZCAPLUS <<LOGINID::20090515>>  
 DN 98:107634  
 OREF 98:16421a,16424a  
 TI Iodine as a reagent for the ready hydrolysis of prop-1-enyl glycosides,  
 for their conversion into oxazolines  
 AU Nashed, Mina A.; Anderson, Laurens  
 CS Dep. Chem., Alexandria Univ., Alexandria, Egypt  
 SO Journal of the Chemical Society, Chemical Communications (1982), (21),  
 1274-6  
 CODEN: JCCCAT; ISSN: 0022-4936  
 DT Journal  
 LA English  
 IT 84766-03-0  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (hydrolysis of, by iodine)  
 RN 84766-03-0 ZCAPLUS  
 CN  $\beta$ -D-Glucopyranoside, 1-propen-1-yl  
 2-deoxy-2-[(1-oxohexadecyl)amino]-, 3-hexadecanoate (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry unknown.